1-Octanol

111-87-5 | DTXSID7021940

## Model Performance

| Model | Data |
|-------|------|

### Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

## Model Results

**Predicted value:** 42.5 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.29e-01

**Confidence level:** 7.28e-01

## Nearest Neighbors from the Training Set

Image not found
1-Octanol
**Measured:** 36.3
**Predicted:** 42.5

Image not found
Ethyl hexanoate
**Measured:** 115
**Predicted:** 110

Image not found
1-Heptanol
**Measured:** 13.8
**Predicted:** 18.6

Image not found
1-Nonanol
**Measured:** 77.6
**Predicted:** 101

Image not found
Ethyl valerate
**Measured:** 93.3
**Predicted:** 68.6